Moving discrete breathers in a Klein–Gordon chain with an impurity

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We analyze the influence of an impurity in the movement of discrete breathers in Klein–Gordon chains. We observe that the moving breather can cross the impurity, can be reflected by it, or can be trapped originating a quasi-periodic breather. We find that resonance with a nonlinear localised mode centred in the impurity is a necessary condition in order to observe the trapping phenomenon, as a difference with the resonance condition with a linear localised mode when this problem is studied within the Nonlinear Schrödinger Equation approximation.

I. INTRODUCTION

A nonlinear phenomena which has been paid a lot of attention during recent years concerns to the localisation of oscillations in discrete nonlinear Klein–Gordon lattices. Since the discovery of intrinsic localised modes or *discrete breathers* by Sievers and Takeno [1], they have been found in a great number of systems. MacKay and Aubry [2] proved the existence of discrete breathers in Klein–Gordon lattices and established a method for calculating them as exact solutions of the dynamical equations (for a review, see [3, 4]). In addition, these localized oscillations, under certain conditions, can move and transport energy and they are usually called *moving breathers* [5, 6, 7, 8, 9].

A method used for calculating discrete breathers in Klein–Gordon lattices consists in approximating the dynamical equations by a Nonlinear Schrödinger Equation (NLS) and the moving breather by an envelope soliton. One problem that had been studied using the NLS limit concerned to the interaction of moving breathers with an impurity supposing that the breather has a small amplitude [10]. However, moving breathers involve oscillations of large amplitude, which implies that the NLS approximation may not be as accurate as expected. The aim of this paper is to study the influence of an impurity in the movement of discrete breathers in a Klein–Gordon chain, i.e. using the dynamical equations without any approximation, a problem which has not been yet undertaken.

In Klein–Gordon lattices, the local modes due to an impurity and the localized modes due to the nonlinearity of the lattice can be considered equivalent entities [11, 12]. This fact suggests that a moving breather can exhibit an interesting behaviour when interacts with an impurity. As a matter of fact, we have found that the moving breather can cross the impurity, can be reflected by it (being able to let the impurity excited), or can be trapped, generating a local depository of energy. The results obtained in our study show that it is necessary the resonance of the moving breather with a nonlinear local mode (i.e. a discrete static breather centred in the impurity site) in order to generate a trapped breather.

This behaviour is qualitatively similar to the observed in the NLS approximation [10]. However, the ranges of the values for which the different phenomena occur are rather different. Furthermore, the most remarkable difference between their approximation and our results is that in they obtained that the trapping is due to a resonance with a linear local mode, whereas in our case, the resonance must involve a nonlinear local mode.

In addition, we have observed the non existence of trapping phenomena even though resonance with the nonlinear local mode occur. We have also observed that in this case the tails of the nonlinear local mode and the lineal local mode have different vibration patterns. As a consequence, we conjecture that both tails must have the same vibration pattern in order that the trapping occur.

II. MODEL AND SOLUTIONS GENERATION

A. Formulation of the model

In order to study the effects of impurities on breather mobility, we consider a simple model where moving breathers can be generated, that is, a Klein–Gordon chain with nearest neighbours attractive interaction [5, 6], whose Hamiltonian is given by:

$$H = \sum_n \left(\frac{1}{2}\dot{u}_n^2 + V_n(u_n) + \frac{1}{2}C(u_n - u_{n-1})^2 \right), \quad (1)$$

where u_n represents the displacement of the n-th particle with respect to its equilibrium position, C is a coupling constant and $V_n(u_n)$ is the on–site potential at the n-th site. We choose V as the Morse potential, i.e., $V_n(u) = D_n(e^{-u} - 1)^2$, which proves to be a very suitable one to obtain moving breathers [6, 7, 9]. D_n represents the well depth in the n-th site. An impurity will be introduced in the chain by means of an inhomogeneity in the 0-th

well, i.e., $D_n = D_o(1 + \alpha\delta_{n,0})$, with α being a parameter which gives account of the magnitude of the impurity. It takes its values in the interval $[-1, \infty)$. Hereafter, we will consider $D_o = 1/2$. Notice that the impurity can be also introduced in the coupling. We have checked that the results are qualitatively the same and will be published elsewhere.

This kind of chain has been used as a simple model of DNA dynamics; in that context it is usually referred to as Peyrard-Bishop model [13]. In the framework of this model, the variables u_n represents the transverse stretching of the hydrogen bonds connecting the two bases, D is the dissociation energy of a base pair, and C is the stacking coupling constant.

This Hamiltonian leads to the dynamical equations

$$F(\{u_n\}) \equiv \ddot{u}_n + V_n'(u_n) + C(2u_n - u_{n+1} - u_{n-1}) = 0. \tag{2}$$

These equations have two kinds of solutions, linear ones, which correspond to oscillations of small amplitude, and nonlinear ones, which correspond to intrinsic localised modes (discrete breathers).

B. Linear modes

The dynamical equations can be linearised if the amplitude of the oscillations is small. Thus, the equations (2) can be written as:

$$\ddot{u}_n + \omega_n^2 u_n + C(2u_n - u_{n+1} - u_{n-1}) = 0, \tag{3}$$

where ω_n is the natural frequency of the n-th oscillator in the harmonic limit. It is related to the well depth of the Morse potential in the form $\omega_n^2 = 2D_n$, which implies that $\omega_n^2 = \omega_o^2(1 + \alpha\delta_{n,0})$, with $\omega_o = 1$ as D_o has been chosen to be $1/2$.

Thus, this equation has $N - 1$ solutions (being N the number of particles) corresponding to linear extended modes (LEMs) and one localised solution, which corresponds to a linear local mode (LLM) whose origin lies in the introduction of the impurity.

The frequencies of the LEMs can be calculated supposing that they are plane waves $(u_n(t) = e^{i\omega(q)t - nq})$ and that the LLM decays in the space following a dependence of the form $u_n(t) = e^{i\omega_L t} r^n$ [10]. Thus, the frequencies of the LEMs are given by:

$$\omega(q) = \sqrt{\omega_o^2 + 4C\sin^2\frac{q}{2}}, \tag{4}$$

where q is the LEM wave vector and takes its value in the interval $(0, \pi]$ if $\alpha < 0$ and in $[0, \pi)$ if $\alpha > 0$.

The frequency of the LLM is given by the relation [10]:

$$\omega_L^2 = \omega_o^2 + 2C + sgn(\alpha)\sqrt{\alpha^2 + 4C^2}. \tag{5}$$

It is worth remarking that LLMs with $\alpha < 0$ have wave vector $q = \pi$ (the particles vibrate in zigzag) while the
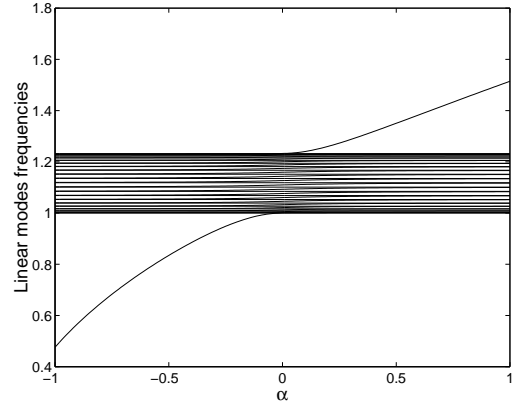

FIG. 1: Frequencies of the nonlinear modes in function of parameter α. They correspond to $C = 0.13$ although the dependence is qualitatively similar for every value of C.

solution for $\alpha > 0$ corresponds to $q = 0$ (the particles vibrate in phase). Figure 1 shows the dependence of the frequencies of the linear modes with α, where the isolated frequencies corresponds to the LLMs.

The knowledge of the frequency of the LLM is very important in order to explain the properties of moving breathers, because discrete breathers and local modes can be viewed as equivalent entities when the interplay between nonlinearity and inhomogeneity is considered [11, 12].

C. Static and moving breathers

A static breather can be obtained solving the full dynamical equations. It can be done using common methods based on the anticontinuous limit [14]. The implementation of these methods basically consists in calculating the orbit of an isolated oscillator at a fixed frequency ω_b, and using this solution as a seed for solving the complete dynamical equations by means of a Newton–Raphson continuation method.

If the oscillator initially chosen is the corresponding to the impurity, a static breather centred in the impurity is obtained. It will be called *nonlinear local mode* (NLLM), in analogy to the linear local modes (LLMs) that appear in the spectrum of linear modes (equation 5).

Once a static breather is calculated, it can be moved under certain conditions. There exists a systematic method to calculate moving solutions [5, 6] which consists in adding to the velocities of the static breather a perturbation of magnitude λ colinear to the direction of the pinning mode, and letting the system evolve in time. This perturbation breaks the shift translational symmetry of the system. In addition, the coupling of the static breather must be strong enough [7].
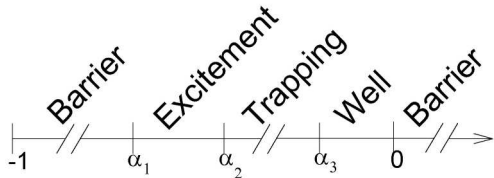
In this paper, we have studied breathers with a fre-

FIG. 2: Different regimes in the interaction of the moving breather and the impurity (see text).

quency $\omega_b = 0.8$ and a coupling $C = 0.13$ although this value has been increased in order to make some comparisons. These values of the parameters provide moving breathers with low phonon radiation for values of the perturbation $\lambda \lesssim 0.2$. We have considered different impurities given by different values of parameter α in the range $-1 \leq \alpha \leq 1$.

III. INTERACTION OF MOVING BREATHERS WITH IMPURITIES

A. Numerical observations

We have studied the behaviour of moving breathers when they interact with an impurity. This study is performed varying the value of the magnitude of the impurity α, and shows an interesting behaviour. We have found some critical values of parameter α ($\alpha_1 < \alpha_2 < \alpha_3 < 0$) which separate the different regimes (see figure 2):

1. *The impurity acts as a potential barrier.* It occurs whenever $\alpha > 0$ and $\alpha \in (-1, \alpha_1)$ with $\alpha_1 < 0$. The breather rebounds when reaches the impurity and let it excited during a brief time lapse. The amplitude of this excitement decreases when the impurity is higher, i.e., when $|\alpha|$ increases. Note that if $\alpha \approx 0$, the potential barrier can be observed, i.e., the breather can cross the impurity provided the translational velocity is high enough, as it occurred in [9].

2. *The impurity is excited and the breather rebounds.* It occurs for $\alpha \in (\alpha_1, \alpha_2)$. The energy of the excited impurity is higher than the energy of the NLLM for the considered value of α and whose frequency is the same as the incident moving breather, ω_b. It implies that the excited impurity will vibrate with a frequency smaller than ω_b because the on–site potential is soft. This behavior is shown in figure 3.

3. *The breather is trapped by the impurity.* It occurs in the interval $\alpha \in (\alpha_2, \alpha_3)$. When the breather is near the impurity, it is absorbed and remains
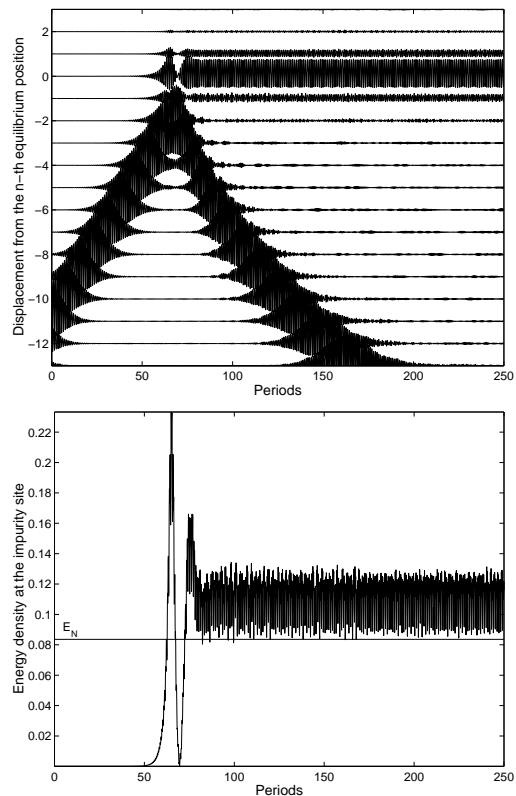

FIG. 3: Interaction of the breather with the impurity for $\alpha = -0.52$ and $\lambda = 0.1$. Top: Evolution of the moving breather. Bottom: Evolution of the averaged energy density of the impurity. E_N is the energy of the NLLM.

trapped while its center oscillates between the neighbouring sites. The trapping of the breather is shown in figure 4. Furthermore, the trapped breather is quasi-periodic, as can be deduced from its Fourier spectrum (Figure 5), and, as a consequence, it emits a great amount of phonon radiation.

4. *The impurity acts as a potential well.* It occurs when $\alpha_3 < \alpha < 0$ and manifests as an acceleration of the breather when reaches a site near the impurity, and a deceleration when the impurity is crossed.

All of these cases have been studied using a breather with $\omega_b = 0.8$ and $C = 0.13$. The translational velocity of the moving breathers has been chosen small so as not to have high phonon radiation. The critical values of α cannot be determined because the transition between the different behaviours are diffuse. An estimation of the critical values for $\omega_b = 0.8$ and $C = 0.13$ are: $\alpha_1 \approx -0.54$, $\alpha_2 \approx -0.49$ and $\alpha_3 \approx -0.02$. These regimes have also been found for different values of the frequency, although the value of α_2 decreases with ω_b.

If the coupling is higher, the phonon radiation is not so low and can mask some of the effects.
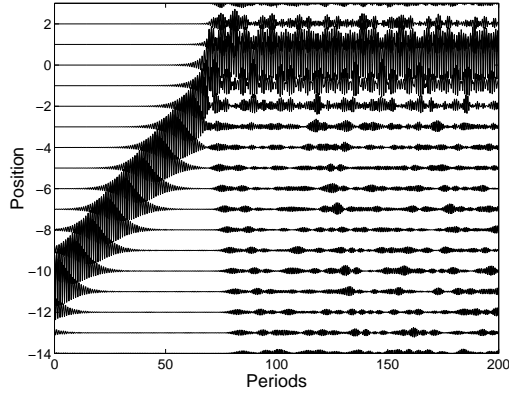
FIG. 4: Evolution of the moving breather for $\alpha = -0.3$ and $\lambda = 0.1$. It can be observed that the breather is absorbed by the impurity and gets trapped; afterwards, the breather emits phonon radiation and its energy centre oscillates between the sites adjacent to the impurity,
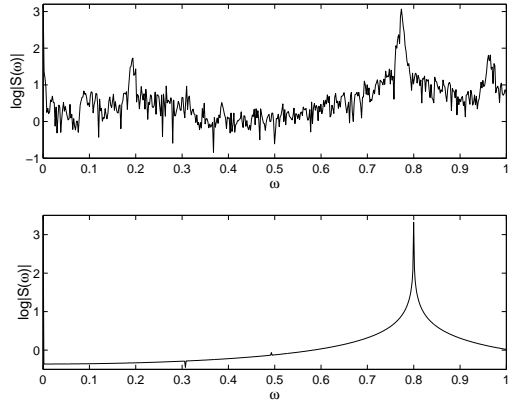

FIG. 5: Fourier spectra for the trapped breather of figure 4 (top) and a static breather with the same values of C and ω_b. It can be observed the existence of only one peak in the last case where there exist a great number of peaks in the first case, which is an evidence of quasi-periodicity.

B. Justification of some results

Some of the results exposed in the last subsection can be explained from the properties of the NLLMs. Concretely, if a continuation of the static breathers is performed varying the parameter α, a bifurcation appears for $\alpha \equiv \alpha_c > 0$ and another one for $\alpha \equiv \alpha_{res} < 0$. The first one is originated by a localized Floquet eigenmode which abandons the unit circle. In the second case, the breather bifurcates with the stationary solution through a pitchfork (figure 6). In this bifurcation, the outer branches correspond to NLLMs either with $u_n > 0$ for $t = 0$ and with $u_n < 0$ for $t = 0$, while the central branch corresponds to the stationary solution, i.e. all the oscillators at rest. This kind of bifurcation is different
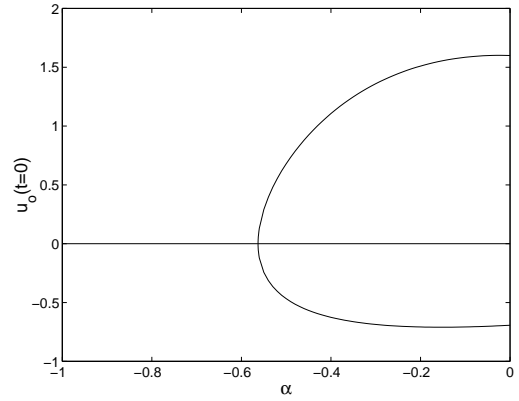

FIG. 6: Pitchfork bifurcation for $\omega_b = 0.8$ and $C = 0.13$. $\alpha_{res} = -0.5328$.

to the broken pitchforks obtained in disordered systems [11, 12, 15]. It is due to the fact that, even thought an isolated impurity breaks the shift translational symmetry of the system, it does not break the mirror symmetry. Consequently, the pitchforks are not broken. The value α_{res} coincides with the point at which the frequency of a LLM is the same as the frequency of the NLLM, i.e., $\omega_L = \omega_b$. This value can be calculated from the equation 5 as a function of ω_b and C:

$$\alpha_{res} = -\sqrt{(\omega_b^2 - \omega_o^2)(\omega_b^2 - \omega_o^2 - 4C)} \qquad (6)$$

Thus, for $C = 0.13$ and $\omega_b = 0.8$, $\alpha_{res} = -0.5628$ which is lower than α_1. We have also checked for different values of the frequency and coupling and we have found that there are situations where α_1 is slightly smaller that α_{res} but always $\alpha_{res} < \alpha_2$. However, the trapped breather does not exist for $\alpha > 0$. It indicates that $\alpha \in (\alpha_{res}, 0)$ is a necessary condition for the existence of the trapped breather.

A conjecture for the existence of trapped breathers when $\alpha < 0$ is the following: in this case, the LLM has $q = 0$, and also all the particles of the NLLM vibrates in phase; this vibration pattern indicates that the NLLM bifurcates from plane waves with $q = 0$ [16], i.e., the NLLM bifurcates from the LLM and it will be the only localized mode that exists when the impurity is excited for $\alpha > \alpha_{res}$. In fact, we have performed successful a continuation from the NLLM to the LLM at constant action and disorder [11, 12]. Thus, when the moving breather reaches the impurity, it can excite the NLLM. However, Doppler effect makes the NLLM 'see' the moving breather with a frequency different from ω_b so that when they interact, they merge into an entity (the trapped breather) with two frequencies.

When $\alpha_{res} < \alpha < \alpha_2$, the NLLM is unable to create a trapped entity. It is observed that the energy of the NLLM decreases with $|\alpha|$, so, there must be threshold for the energy of the NLLM in order that the trapped

breather can exist. The narrow window of impurity excitements observed in the interval (α_1, α_2) can be due to a resonance of the moving breather with the NLLM of frequency slightly smaller that ω_b and, therefore, the excited impurity has a higher energy than the NLLM of frequency ω_b, as we are considering a soft potential.

For $\alpha < \alpha_{res}$, the trapped breather cannot be generated, and the moving breather always rebounds. In addition, the NLLM does not exist. Therefore, there must be connection between both facts, i.e., the existence of the NLLM will be a necessary condition in order to obtain a trapped breather.

If $\alpha > 0$, the scenario is different. In this case, the LLM has $q = \pi$ but the NLLM's particle vibrate again in phase, that is, the NLLM will not bifurcate from the LLM. Thus, there are two different localized modes for $\alpha > 0$: the LLM and the NLLM. But, actually, the equations that govern the system are nonlinear, so the linear modes can only correspond to low-amplitude oscillations. In the case of the NLLM, the linear regime corresponds to the tails. Thus, if the moving breather reaches the impurity site, it will excite the NLLM, its tails and also the tails of the LLM. But the latter vibrate in zigzag. As a consequence, there will be two different linear localized entities: the tails of the LLM (vibrating in zigzag) and the tails of the NLLM (vibrating in phase). Therefore, we conjecture that the existence of both linear localized entities at the same time may be the reason why the impurity is unable to trap the breather when $\alpha > 0$.

To summarize, the existence of a NLLM for a certain value of α is necessary for the existence of trapped breathers. However, if there exists a LLM with a different vibration pattern to the NLLM, the trapped breather does not exist.

IV. CONCLUSIONS

We have studied the interaction of a moving discrete breather in a Klein–Gordon chain with an impurity at rest. A rich behaviour is observed when the breather reaches the impurity. It can be summarized as follows: a) the impurity can act as a potential barrier or a potential well; b) the breather can be reflected by the impurity which is let excited; c) the impurity can trap the breather, making it quasi-periodic.

A previous work made using the NLS approximation

[10] showed that moving breathers interacting with an impurity have qualitatively the same behaviour as the observed by us. There is, however, a very important difference between this work and ours. It relies in the fact that in the NLS approximation, a resonance between the frequencies of the moving breather and the linear local mode created by the impurity is needed whereas in our case, this resonance prevents the breather from being trapped. In our case, the trapping phenomena is owed to the resonance between the moving breather and a nonlinear localised mode.

The model used in our study is the same as the studied by Peyrard and Bishop to explain DNA denaturation [13]. It indicates that our results can be applied to study some properties of DNA chains. For instance, if a moving breather is generated in a DNA chain, it can be trapped by an impurity, and act as a precursor of the transcription bubble [17]. This trapped breathers can interact with another breathers and collect energy [18].

The impurity in DNA can have two different origins. The first one consists in a modification of the well depth due to the action of a transcription enzyme through a chemical effect, as explained in [17]. The second one relies in the fact that the A-T base pairs have 2 hydrogen bonds whereas the C-G base pairs have 3 hydrogen bonds. So, it can be supposed that in the first case, the well depth of the Morse potential is 2/3 of the second case. From the results of this paper, trapping does not occur when the well depth in the impurity is higher than in the homogeneous area. It implies that trapping can occur in a chain of C-G pairs with an impurity of A-T. Nevertheless, the main fault of these mechanisms is the assumption of homogeneity in DNA, where the role of the inhomogeneity due to the genetic code is known to be crucial in the dynamics [19]. However, the study of the effects of impurities is the first step to understand the dynamics of moving breathers in DNA sequences.

[1] A. Sievers and S. Takeno, Phys. Rev. Lett. **61**, 970 (1988).

[2] R. MacKay and S. Aubry, Nonlinearity **7**, 1623 (1994).

[3] S. Flach and C. Willis, Physics Reports **295**, 181 (1998).

[4] S. Aubry, Physica D **103**, 201 (1997).

[5] D. Chen, S. Aubry, and G. Tsironis, Phys. Rev. Lett. **77**, 4776 (1996).

[6] S. Aubry and T. Cretegny, Physica D **119**, 34 (1998).

[7] J. Cuevas, J. Archilla, Y. Gaididei, and F. Romero, Physica D **163**, 106 (2002).

[8] M. Ibañes, J. Sancho, and G. Tsironis, Phys. Rev. E (2002), in press.

[9] J. Cuevas, F. Palmero, J. Archilla, and F. Romero, Phys. Lett. A (2002), submitted.

[10] K. Forinash, M. Peyrard, and B. Malomed, Phys. Rev. E **49**, 3400 (1994).

[11] J. Archilla, R. MacKay, and J. Marín, Physica D **134**, 406 (1999).

[12] J. Cuevas, J. Archilla, F. Palmero, and F. Romero, J. Phys. A: Math. Gen. **34**, L1 (2001).

[13] M. Peyrard and A. Bishop, Phys. Rev. Lett. **62**, 2755 (1989).

[14] J. Marín and S. Aubry, Nonlinearity **9**, 1501 (1996).

[15] G. Kopidakis and S. Aubry, Physica D **130**, 155 (1999).

[16] S. Flach, Physica D **91**, 223 (1996).

[17] J. Ting and M. Peyrard, Phys Rev E **53**, 1011 (1996).

[18] O. Bang and M. Peyrard, Phys. Rev. E **53**, 4143 (1996).

[19] M. Salerno and Y. Kivshar, Phys. Lett. A **193**, 263 (1994).